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An order parameter equation for non-linear rheology of dense colloidal suspensions

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ガラス物質は、高温低密度状態で剪断応力がshearに対して線形に増加するNewton則がみられるが、低温高密度状態になるとshear-thinning、shear-thickening、降伏応力の発生などの、応力がshearに対して非線形な応答をする現象が見られる。これらの非線形レオロジーに関して、実験・シミュレーション・MCTを用いた解析計算によって様々な研究がなされてきた。しかし、ガラス 状物質の非線形レオロジーの完全な理解は未だになされていない。このような錯綜した状況の中で、ガラス状物質のレオロジー特性を統一的に理解するために、コロイド分散系のレオロジー特性を微視的なモデルから導出した。

1 Introduction

Materials with a large relaxation time are called as "glassy materials". They include polymers, emulsions and colloidal suspensions as well as usual molecular glass. It has been known that that the rheological properites of glassy materials strongly depend on the density and the temperature of the materials. At a high temperature and low density state, the shear stress σ_{xy} behaves as a linear function of the shear rate γ. On the contrary, at a low temperature and high density state, the shear stress σ_{xy} behaves as a non-linear function of the shear rate γ. In this state, intriguing phenomena such as shear thinning, shear thickening and the appearance of yield stress are observed. Although the rheological properties of glassy materials have been studied by experiments, simulations and theoretical approaches, a systematic understanding of them is not obtained yet.

2 Approach

Recently, aiming at understanding the rheological properties of glassy materials, we have derived the equation which describes the relation between σ_{xy} and γ in colloidal suspensions from a microsopic model (e-print: cond-mat/ 0511111). In colloidal suspensions, the stress σ_{xy} is determined from the pair distribution function $g(\mathbf{r})$. From this simple fact, we obtain an order

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parameter equation that describes the rheological properties by applying a bifurcation analysis to an evolution equation for the pair distribution function $g(\mathbf{r})$ under some approximations.

3 Result

We drive the equation

$$a(T - T_s)\sigma_{xy} + b\sigma_{xy}^3 + c\gamma = 0, \tag{1}$$

where T is the temperature of the system, and a, b, c and T_s are constants which can be calculated from the interaction potential between colloidal particles. Clearly, one can find the similarity of Eq. (1) with the Ginzburg-Landau equation for ferromagnetic materials, where the shear stress σ_{xy} and the shear rate γ correspond to the magnetization M and the external magnetic field H, respectively.

In the left hand of the figure 1, the relation between σ_{xy} and γ is demonstrated by using Eq. (1). One can see the following behavior:

1. When $T > T_s$, σ_{xy} is proportional to γ at low shear rate. At high shear rate, σ_{xy} is proportional to $\gamma^{1/3}$.

2. When $T = T_s$, σ_{xy} is proportional to $\gamma^{1/3}$ at all shear rate.

3. When $T < T_s$, σ_{xy} has a finite value (dynamic yield stress) in the limit $\gamma \to 0$.

These behaviors are also observed in numerical experiments of molecular dynamics simulation, as shown in the right hand of the figure 1.

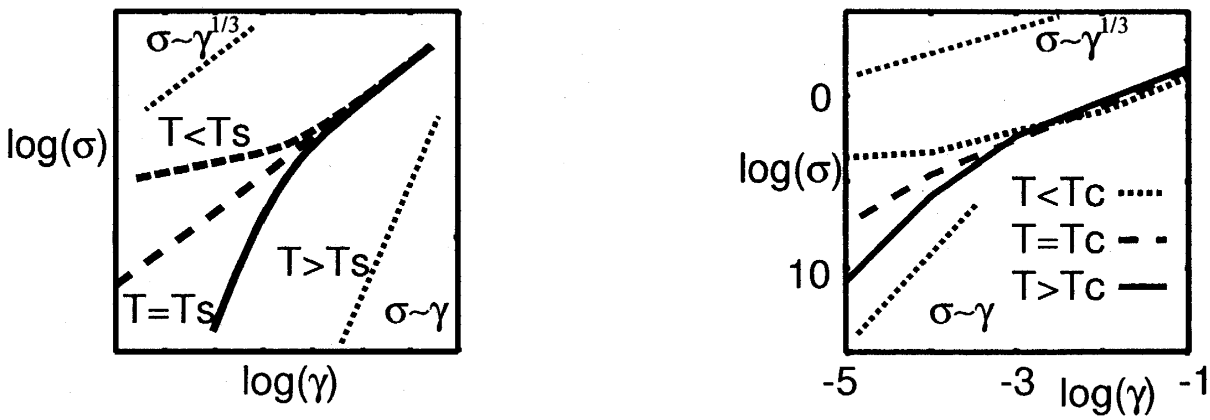

Figure 1: Shear stress σ_{xy} as a function of the shear rate γ. Left: Result of Eq. (1). Right: Result of the numerical experiments.